12

RESEARCH AND DEVELOPMENT OF METHODS FOR ESTIMATING PHYSICOCHEMICAL PROPERTIES OF ORGANIC COMPOUNDS OF ENVIRONMENTAL CONCERN

FINAL REPORT ON PHASES I-IV

by

Warren J. Lyman, Ph.D.

June 1982

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This report summarizes the four-year program undertaken to evaluate, and provide information on, estimation methods for environmentally-important properties of organic chemicals. The work was conducted in four phases. Phase I was a problem definition study to identify those physicochemical properties that are most needed for assessments of a chemical's environmental fate and transport, and to determine which of these properties were estimable. In Phase II, the available estimation methods for 26 properties were evaluated and described in a 1000-page handbook. Clear recommendations and instructions were provided for

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the use of all methods. Phase III included several modifications to the Phase II handbook to facilitate commercial publication. No formal government report was published for the Phase III work. In Phase IV, an interactive computer system (CHEMEST) incorporating several property estimation methods from the handbook was designed and implemented.

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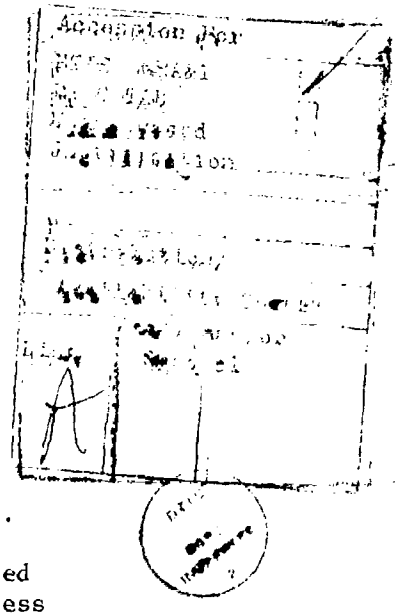

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The original idea for this program was by our Project Officer, Dr. David H. Rosenblatt of the U.S. Army Medical Bioengineering Research and Development Laboratory (Fort Detrick, Frederick, MD). He had the vision to see the critical need for this work and the skills to see that a program was initiated. His initiative, guidance, and scientific and editorial skills were essential to the successful completion of the program.

The U.S. Army Medical Bioengineering Research and Development Laboratory funded the Phase I study, a major portion of the Phase II study, all of the work in Phase III, and a significant portion of the Phase IV work. Financial support for Phase II was also provided by the U.S. Army Toxic and Hazardous Materials Agency (Aberdeen Proving Ground, MD) and the U.S. Environmental Protection Agency's Office of Pesticides and Toxic Substances (Washington, D.C.).

Many individuals in Arthur D. Little, Inc., the US Army, the Environmental Protection Agency, and in various Universities contributed to the successful completion of this program. Specific credits are provided in the publications and reports prepared at the end of each Phase.

Warren J. Lyman
Program Manager
Arthur D. Little, Inc.

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1. OVERVIEW

During the preparation, in 1977-78, of Problem Definition Studies on toxic chemicals of interest to the US Army, it became clear that timely and complete environmental assessments could not be made for several chemicals because of numerous physicochemical property data gaps. Basic properties such as water solubility, vapor pressure, and bioconcentration factors were needed to assess the probable environmental partitioning, transport and degradation of these chemicals.

It was also realized that many of these properties could be estimated with accuracies sufficient for environmental assessments. Some of the estimation methods (e.g., for boiling points) had existed in the literature for many years, while others, primarily those dealing with "environmental properties" (e.g., bioconcentration factors), had been developed only recently and were widely scattered in the literature. What was clearly needed was a report or handbook that would provide environmental scientists and managers with a compilation of such estimation methods, with clear recommendations and instructions for their use. This program was designed to satisfy that need.

The program was carried out in four Phases, as follows:

Phase I: Problem Definition Study

Dates: September 1978 - February 1979

Objectives: (1) To identify those physicochemical properties (of organic compounds) that are most needed for assessments of the environmental fate and transport; and (2) to determine which of these properties could be estimated with available methods.

Output: The Phase I report [1]* identified over 40 properties or parameters of interest. Of these, 24 were found to be estimable.

Phase II: Preparation of Estimation Methods Handbook

Dates: May 1979 - June 1981

* References are provided in Section VI.

Objective: To prepare a handbook of chemical property estimation methods for 26 environmentally-important properties of organic chemicals.

Output: The Phase II report [2] provided the desired quantitative chemical property estimation methods for 24 properties, with clear recommendations and instructions for their use. Chapters were included on 2 properties for which only qualitative predictions could be made.

Phase III: Commercial Publication of Handbook

Dates: January 1981 - May 1982

Objective: To modify the Phase II report (handbook), including the addition of a subject index and permission statements covering copyrighted material, to allow publication by a reputable publisher. A commercial publication was needed to insure the widest possible dissemination of this work.

Outputs: (1) A Publishing Agreement [3] between Arthur D. Little, Inc., and McGraw-Hill Book Co. was signed in October 1980; (2) a letter-style Phase III report [4] was submitted in September 1981; and (3) the McGraw-Hill Handbook of Chemical Property Estimation Methods [5] was published in May 1982. Note that there was no formal government report published under Phase III, only an unpublished letter-style report [4].

Phase IV: Design and Implementation of a Computerized Chemical Property Estimation System

Dates: September 1981 - July 1982

Objective: To design and implement a computerized, interactive chemical property estimation system incorporating selected property estimation routines from the Phase II handbook.

Outputs: A computer system, CHEMEST, was designed and implemented on a VAX 11/780 owned by the U.S. Environmental Protection Agency [6]. A User's Guide [7] and a Programmer's Maintenance Manual [8] for CHEMEST were prepared.

The work in each of these Phases is described in additional detail in Sections 2 - 4 of this report. Recommendations for future work are given in Section 5.

The U.S. Army Medical Bioengineering Research and Development Laboratory (Fort Detrick, Frederick, MD) provided the leadership for most of this four-year program. Phases I - III were carried out under Contract No. DAMD17-78-C-8073 and Phase IV under Contract No. DAMD17-81-C-1179. Inter-agency funding from the U.S. Army Toxic and Hazardous Materials Agency (Aberdeen Proving Ground, MD) and the U.S. Environmental Protection Agency's Office of Pesticides and Toxic Substances (EPA/OPTS) (Washington, D.C.) provided partial support for work conducted in Phase II. The EPA/OPTS provided a major portion of the funding for Phase IV through a separate EPA contract. The EPA also took a leadership role in Phase IV with regard to: (1) overall system design for CHEMEST; (2) the selection of properties to be included with the EPA portion of the funding; and (3) the system documentation.

2. PHASE I

The Phase I program was, essentially, a problem definition study to develop a ranked list of properties or parameters to be included in the handbook. The ranked list of properties was developed following an analysis of the physicochemical properties required in environmental transport and fate models, legally mandated lists of chemicals and properties, hazard and ranking schemes, and other pertinent material (including expert opinion). The rank of each property was based upon a consideration of its general importance and frequency of occurrence in the models, ranking schemes, and regulations, etc.

The Phase I program identified over 40 properties or parameters (associated with environmental concerns of organic chemicals) for which estimation techniques are desirable. However, estimation techniques having some degree of general applicability appeared to be available for a little over half of these properties. These are listed as numbers 1-25 in Table 1. Also listed in Table 1 (nos. 26 and 27) are two additional properties, rates of biodegradation and rate of aqueous photolysis, which were qualitatively discussed in the Phase II handbook even though reliable (or generally applicable) estimation methods are not currently available for these properties. These two properties are considered to have a ranking equal to the estimable properties at the top of the list in Table 1. Their addition to the list of properties to be considered in Phase II reflects not only this high ranking, but also the specific interests and needs of the federal agencies who contributed to the support of the Phase II work.

The Phase I report [1], in addition to documenting the identification and ranking of the properties of interest, also provides an overview of the available estimation techniques, a general description of recent work in the area of environmental fate modeling, and a bibliography of articles, reports and books that were collected for review.

TABLE 1

ESTIMABLE PROPERTIES IDENTIFIED IN PHASE I

1. Solubility in Water
2. Vapor Pressure
3. Octanol/Water Partition Coefficient
4. Adsorption Coefficient
5. Bioconcentration Factors
6. Rate of Volatilization from Water
7. Rate of Hydrolysis
8. Dissociation Constant
9. Activity Coefficient
10. Rate of Volatilization from Soil
11. Diffusion Coefficient in Air[a]
12. Diffusion Coefficient in Water[a]
13. Density of Gases, Liquids and Solids
14. Boiling Point
15. Heat of Vaporization
16. Flash Point
17. Solubility in Other Solvents
18. Surface Tension
19. Interfacial Tension with Water
20. Viscosity of Liquids
21. Heat Capacity of Gases and Liquids
22. Thermal Conductivity of Liquids
23. Atmospheric Residence Time
24. Dipole Moment
25. Refractive Index
26. Rate of Biodegradation[b]
27. Rate of Aqueous Photolysis[b]

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a. Properties 11 and 12 were combined in a single chapter.

b. Quantitative estimation methods not currently available. (See text.) These properties have a high ranking based on information needs.

3. PHASE II

The major work in Phase II consisted of additional literature searches (for estimation methods for the selected properties), the evaluation of estimation methods, and the preparation of the Phase II report [2]. The report thus contains selected estimation methods for several environmentally important physicochemical properties of organic chemicals. The general style of the report is that of a handbook with specific instructions for the use of each estimation method.

Table 2 provides a summary of the contents of the 1000-page Phase II report. Because of the length of the report, it was separated into two parts for printing and subsequent ease of handling.

Each of the 26 chapters of this handbook covers one physicochemical property or parameter. With few exceptions, each chapter provides: (1) a general discussion of the property and its importance in environmental considerations, (2) an overview of available estimation methods, (3) a description plus step-by-step instructions for each selected method, (4) worked-out examples for each method, (5) a listing of sources of available data on the property, (6) a list of symbols used, and (7) the cited references. The chapters on Rate of Aqueous Photolysis (Chap. 8) and Rate of Biodegradation (Chap. 9) depart from the usual format and provide only qualitative or semiquantitative information; neither of these properties can be estimated at present.

Most chapters provide two or more estimation methods. In selecting the methods, we favored those that: (1) are applicable to a variety of chemical classes and structures, (2) are relatively simple to use with no more than a desk calculator, (3) require a minimum of input data; and (4) are reasonably accurate. Information on method errors is provided with each chapter; an appendix describes a procedure to estimate propagated and total error in situations where one or more inputs must first be estimated. None of the selected methods is intended to be applicable to organic mixtures, polymers, solutions, or inorganic compounds.

TABLE 2

SUMMARY OF CONTENTS OF PHASE II REPORT

PART 1

Executive Summary
Acknowledgments
Table of Contents
List of Tables
List of Figures
Introduction
1 — Octanol/Water Partition Coefficient
2 — Solubility in Water
3 — Solubility in Various Solvents
4 — Adsorption Coefficient for Soils and Sediments
5 — Bioconcentration Factor in Aquatic Organisms
6 — Acid Dissociation Constant
7 — Rate of Hydrolysis
8 — Rate of Aqueous Photolysis
9 — Rate of Biodegradation
10 — Atmospheric Residence Time

PART 2

11 — Activity Coefficient
12 — Boiling Point
13 — Heat of Vaporization
14 — Vapor Pressure
15 — Volatilization from Water
16 — Volatilization from Soil
17 — Diffusion Coefficients in Air and Water
18 — Flash Points of Pure Substances
19 — Densities of Vapors, Liquids and Solids
20 — Surface Tension
21 — Interfacial Tension with Water
22 — Liquid Viscosity
23 — Heat Capacity
24 — Thermal Conductivity
25 — Dipole Moment
26 — Index of Refraction

Appendix A — Bibliography of Standard Chemical Property Data Sources

Appendix B — Simple Linear Regression

Appendix C — Evaluating Propagated and Total Error in Chemical Property Estimates

Appendix D — Recommendations for Future Research and Development

Our goal in this program was to distill the widely scattered literature, much of recent origin, in order to select and present in an organized manner the most appropriate estimation methods for particular chemical properties. This information should be useful to environmental chemists, environmental program managers, and even some chemical process engineers, who must frequently deal with problematic chemicals for which even the most basic physicochemical properties may be unknown. The methods described permit rapid estimation of properties and thereby facilitate studies of these problematic chemicals for such purposes as chemical fate modeling, exposure assessments, priority ranking of large lists of chemicals, and process design.

The successful management of the Phase II program (resulting in the preparation of the 1000-page estimation methods handbook) was helped by many factors, not the least of which was the clear support and high standards of the Project Officer. Two other factors should be mentioned. One was the use of a problem definition study (Phase 1) which allowed us to prepare a very detailed scope of work for Phase II. The second was the preparation, early in Phase II, of detailed instructions, budgets and time schedules for each author. A 14-page "Format and Style Instructions" report was prepared with guidance from our professional editor (W. Reehl). These instructions detailed the outline for each chapter, format and style for tables, equations, references, symbols, and other features. Sample pages were also included along with several examples of references. Special attention was given to type sizes, fonts and margins so that the Phase II mats could be used directly (with up to 20% reduction) by the commercial publisher chosen in Phase III.

Special mention should be made of the quality control procedures used in the preparation of the handbook. The normal steps in the preparation of each individual chapter were as follows:

(1) The preparation of an initial draft by the author;

(2) A review for general completeness by the Project Manager (W. Lyman); significant revisions were often required;

(3) In-depth editing by a professional editor with over thirty years of experience in technical writing and editing (W. Reehl);

(4) Entering the text into a DECSET word processing system (art, equations, tables and examples were composed on stand-alone typewriters) with subsequent proofing by professional proofreaders, the editor and the author. Two or three iterations were usually required to obtain a clean, fully-composed draft.

(5) Simultaneous reviews of the draft by:

a) The Project Officer (D. Rosenblatt), who also served as editor;

b) An internal (A.D. Little) reviewer selected by the author;

c) An external reviewer (generally from the U.S. EPA or a university) also selected by the author;

d) Other interested individuals in the U.S. Army and the U.S. EPA;

(6) The consideration of all reviewer's comments and the preparation, by the author, of a revised chapter which was again edited by the professional editor;

(7) Review of the revised draft by the Project Manager, the Project Officer and the National Bureau of Standards*, with subsequent revisions as required.

(8) A final review of the whole handbook when submitted as a draft final report.

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* The National Bureau of Standards (NBS) conducted a separate review of several handbook chapters under contract to the U.S. EPA. Because of time and financial constraints, we were unable to incorporate many helpful suggestions from the NBS; all errors were, however, corrected.

This process, especially the use of a professional editor and the preparation of composed material prior to the in-depth technical review, was found to be very supportive of the quality control efforts.

4. PHASE III

In Phase III we modified the Phase II Final Report of this contract in order to prepare a final manuscript (type-set copy with fully rendered illustrations) for publication. After consideration of several publishing firms, McGraw-Hill Book Co. (New York, NY) was chosen as the publisher because of its solid reputation and its willingness to publish at a reasonable price. The McGraw-Hill version [5] has been entitled: HANDBOOK OF CHEMICAL PROPERTY ESTIMATION METHODS, and subtitled: Environmental Behavior of Organic Compounds. Warren J. Lyman, William F. Reehl and David H. Rosenblatt are listed as editors.

Major elements of the Phase III work involved:

- The negotiation of a Publishing Agreement [3] with McGraw-Hill Book Company;
- The preparation of a subject index for the book (to replace Appendix D in the Phase II report);
- Revisions to the Acknowledgements, Introduction and other portions of the front matter of the Handbook;
- Obtaining permission from other publishers and - where required - other authors to reproduce previously copyrighted material;
- The removal of the A.D. Little logo and the addition of running heads for every page in the Handbook; and
- Significant revisions to Chapter 11 (Activity Coefficient) to incorporate more up-to-date information on the UNIFAC method.

Work on Phase III was mostly completed by early September 1981. The camera-ready originals for the Handbook were sent to McGraw-Hill Book Co. on August 17, 1981; a copy of all copyright permission letters were sent to them - per the Publishing Agreement between Arthur D. Little and McGraw Hill - on September 9, 1981. A few final corrections to the mats were made in February 1981. The book completed its first-run print in May 1982.

All royalties from the McGraw-Hill Book Co. sales will go to a not-for-profit foundation specially created to insure that future revised editions of the handbook are prepared.

5. PHASE IV

The purpose of Phase IV was to design and implement an interactive computer system containing selected property estimation routines from the Phase II handbook. The system, called CHEMEST, currently includes estimation methods for the following properties:

		No. of Estimation Methods in CHEMEST
1.	Water solubility[a]	4
2.	Soil adsorption coefficient	4
3.	Bioconcentration factors for fish[b]	3
4.	Activity coefficients for binary systems[b]	2
5.	Boiling point	7
6.	Vapor pressure	3
7.	Rate of volatilization from water[b]	2

It is expected that additional EPA funding will allow other properties to be added in the near future. A User's Guide and a Programmer's Maintenance Manual for the existing system have been prepared [7,8].

It is the primary objective of CHEMEST to provide users with technical assistance--and rapid, calculation-error-free estimates--associated with the prediction of environmentally-important properties of organic chemicals. Technical assistance is provided to users of CHEMEST not only by the computerization of all calculations, but by a variety of other features of the system including prompts and requested prompts (to provide more information about required inputs) that are described below. CHEMEST is designed to be used by individuals with at least one year of organic chemistry. Training for the use of the computer system itself is expected to require about one day; less for those that are already familiar with the estimation methods used.

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a. Partly funded by Contract No. DAMD17-81-C-1179

b. Funded by Contract No. DAMD17-81-C-1179.

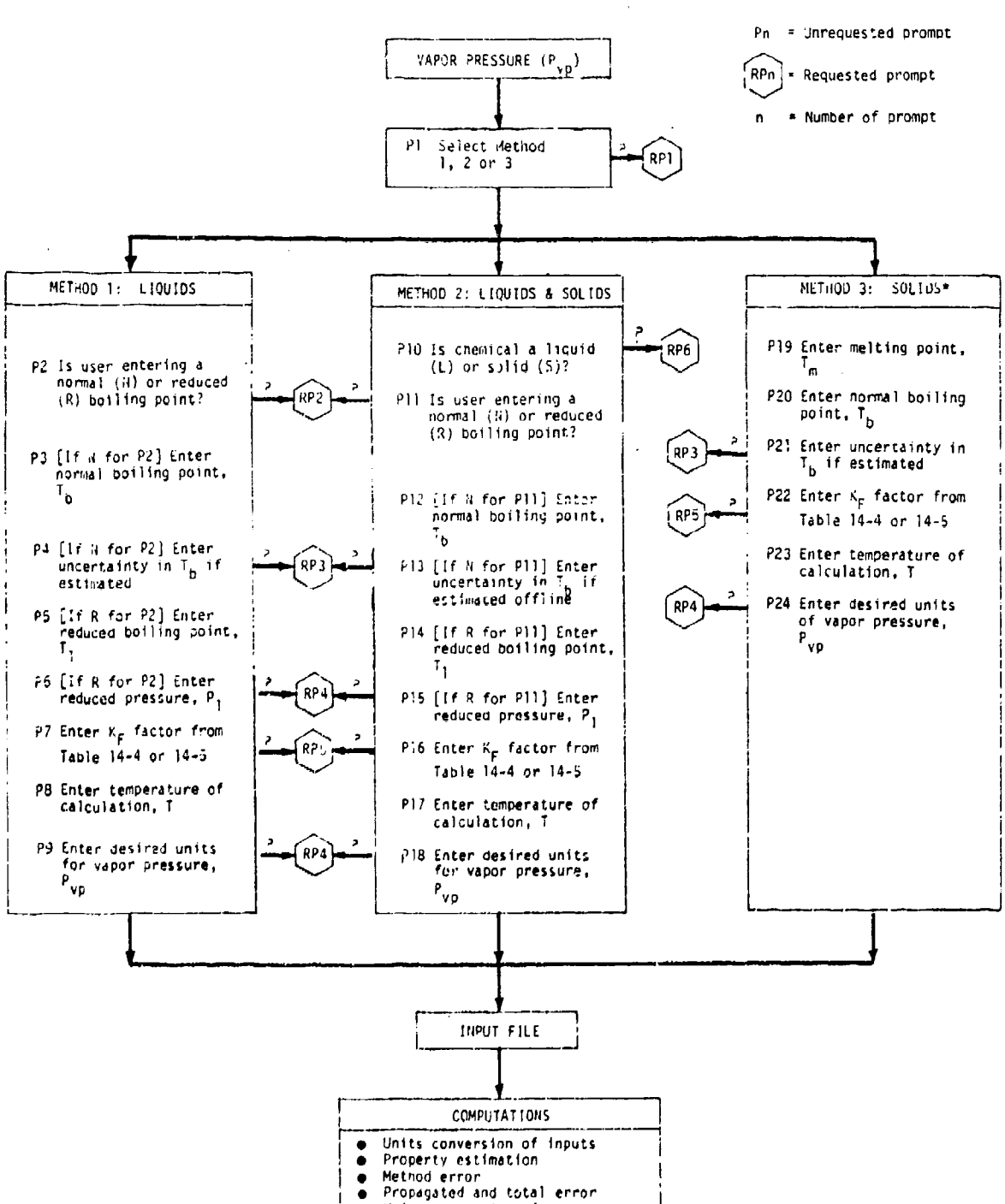
Key Features of the System

CHEMEST is a fully interactive, user-friendly system which may be used with most kinds of computer terminals (video or hardcopy). Upon entering the system, a series of prompts--and requested prompts--helps guide the user to the property of interest, to the appropriate method(s) for the property, and to input the needed information for the chosen method. Figure 1 shows, for example, a flowchart for the interactive portion of the vapor pressure estimation routine. At each place (prompt) where it appears possible that some users may be confused or require additional help, additional information (a requested prompt) may be called up by typing '?' in response to the initial prompt. The requested prompts may supply explanatory text, tables of values that might be used as default values for certain constants, and/or examples of just what is required for input.

There is no chemical property data file currently associated with CHEMEST; all inputs must be supplied by the user in the interactive portion of the run. However, the system does contain a state file of user-supplied inputs so that--until a new chemical is specified--the user need not re-enter any property already entered. For example, if the user wished to compare the results of Methods 2 and 3 for the estimation of a chemical's vapor pressure, the inputs for Method 2 (T_b, K_F, T, and desired output units; cf Figure 1) would be entered and an estimate obtained. The user would next specify Method 3; the only new entry required is T_m. The other inputs previously entered for Method 2 can be changed, if desired, but need not be re-entered otherwise. If a value for the boiling point (T_b) had previously (in this run) been estimated by CHEMEST, this estimate would be in the state file and available for automatic recall.

Another key feature of CHEMEST is the inclusion of information on method error, and the ability--for key inputs--to automatically calculate the propagated and total error in the final estimate when the key input was itself an estimate with some method error. The method

FIGURE 1. FLOWCHART FOR CODED METHODOLOGY: VAPOR PRESSURE



errors assigned in CHEMEST are derived from comparisons of experimental and estimated values for a set of chemicals. In some cases (e.g., for vapor pressure) the assigned method error is a function of the value of the estimate.

For convenience, CHEMEST allows the user to input data in a variety of common units and to select different units for the estimate to be supplied. The output file given after each estimation run includes not only the desired estimate, but also the method and total errors associated with the estimate, a summary listing of the key inputs, and the method number and (ADL Handbook) equation numbers used. At the user's, request, the output will display the values of other user-supplied inputs.

CHEMEST has a system command mode that allows the user to exit from almost any portion of the interactive sequence. The exit may be to obtain a requested prompt on system commands, to specify a new chemical property or estimation method, or to restart the current method. This feature helps save the user's (and computer's) time by not forcing the completion of all inputs in cases where the user desires to exit for any reason.

For advanced users, CHEMEST includes a special 'CHANGE' command that allows the value of any input to be specified (or changed if a value had been previously entered) without having to go through the normal sequence of prompts. This will facilitate repeat calculations where one--or just a few--inputs are being varied, and will make possible future linkage with the batch input of data.

Program Coding, Hardware, and Documentation

CHEMEST is coded in ANSI standard Fortran using non-restrictive code that is readily adaptable to computers of different manufacturers. It is installed on a VAX 11/780 owned by the U.S. government. The coding is heavily documented to allow subsequent changes and additions. In addition, a User's Guide [7] and Systems Maintenance Manual [8] have been prepared.

CIS Interface

At the completion of this project, a copy of the CHEMEST program and associated documentation will be made available to the NIH/EPA Chemical Information System (CIS). Users with CIS access will thus be able to use CHEMEST on the CIS computer system. No time frame for the CIS-implementation of CHEMEST has been established.

6. RECOMMENDATIONS

There are two key recommendations that are directed to all agencies and organizations that have an interest in chemical property estimation:

1. The estimation methods handbook should be revised, updated and expanded periodically.

2. The computerized chemical property estimation system, CHEMEST, should be expanded to cover additional properties and updated periodically.

Handbook Revisions

Appendix D of the Phase II report [2] contains detailed recommendations on future revisions that appear desirable for each of the 26 existing handbook chapters. It also lists additional properties - not covered by the handbook - that should be included in future editions if estimation methods are available. Table 3 provides a summary list of properties for which estimation methods are desirable. Of the 20 properties listed, we note that about 12 are probably estimable and would be candidates for new chapters in the next handbook edition.

In addition to the above, it may be desirable to consider other expansions of the handbook to cover t e properties of mixtures, polymers, solutions, and inorganic compou d .

The amount of work (and req nding) for the preparation of a revised and expanded handbook should not be underestimated. Many of the chapters in the existing handbook will require major revisions. The types of work required for these chapters include: (1) a review of the literature since 1979; (2) the evaluation and addition of new methods; and (3) a more detailed and rigorous evaluation of all methods with regard to method errors and extent of applicability to different chemical classes. Based on the experience gained in this program, we

estimate that the average cost (in 1980 dollars) of each new chapter would be about $15,000; a major revision to an existing chapter would be about $10,000; a series of minor revisions to a chapter about $5,000.

Significant cost savings could be achieved if new or revised chapters were prepared by individuals (to whom a modest per-page fee was paid) rather than via contract with a consulting firm. However, the loss in management control might prove a serious problem. In addition, we expect that the commercial publisher would take over the typesetting of future editions with some associated cost savings. Finally, as noted in Section 4, some funds will be available from royalty payments associated with the McGraw-Hill Sales of the existing editions.

We would recommend that a revised and expanded handbook be published no later than 1987. To achieve this goal, detailed planning should start no later than January 1984, and the actual work no later than January 1985.

TABLE 3

PHYSICOCHEMICAL PROPERTIES FOR WHICH ESTIMATION METHODS ARE DESIRED

PARTITIONING WITH AIR

(1) Henry's Law Constant* (air/water partition coefficient).

(2) Vapor/aerosol partition coefficient (describing adsorption (or absorption) of organic vapors onto (into) atmospheric aerosols).†

BIODEGRADATION

(3) Rates of biodegradation under the most important conditions.†

BIOCONCENTRATION

(4) Rates of (a) uptake and (b) clearance (and metabolism) by aquatic life.†

(5) Bioconcentration factors for terrestrial organisms, both plants and animals.†

ADSORPTION/SOIL TRANSPORT

(6) Rates of (a) adsorption and (b) desorption on soils and sediments.

(7) Adsorption coefficients for adsorption on minerals (e.g., sand and clay) that are low in organic carbon content.

(8) Adsorption coefficient for desorption process when hysteresis is present.

(9) The exponential coefficient, n, in the Freundlich (adsorption) isotherm equation.

(10) Apparent diffusion coefficient in soils.†

REACTIVITY

(11) Rate of aqueous photolysis (including absorption spectra above 290 nm and quantum yields).

(12) Rate constants for reaction, in the atmosphere, with (a) OH radicals, (b) ozone, and (c) light.†

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*Acceptable estimation methods for this property are currently available.

†Some estimation methods exist for these properties, but their validity and range of applicability have not been assessed.

TABLE 3 (continued)

REACTIVITY

(13) Rate constants for reaction, in water, with (a) free radicals and (b) other oxidants.†

(14) Reactivity with common materials of construction.

ENVIRONMENTAL TRANSPORT

(15) Deposition velocities for use in assessing air-to-ground (and air-to-surface water) transport pathways. Both wet and dry fallout must be considered.†

OTHERS

(16) Flammability limits in air.

(17) Melting point.†

(18) Heat of fusion.†

(19) Heat of solution.

(20) Heat of combustion.†

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* Acceptable estimation methods for this property are currently available.

† Some estimation methods exist for these properties, but their validity and range of applicability have not been assessed.

CHEMEST Revisions

The CHEMEST system currently contains computerized estimation routines for seven properties. (Some additional EPA funding is expected to allow the inclusion of at least two more property routines.) Specific recommendations for CHEMEST are to:

1) Expand the system to cover additional properties covered by the handbook.

2) Revise existing routines as revised editions of the handbook are prepared.

3) Include in the system a means for the user to input a chemical's structure (e.g., via Wiswesser Line Notation (WLN), connectivity table, or the drawing of the structure on a video terminal). The structural information would then be linked automatically with all fragment constant methods and relieve the user of any additional structural inputs.

4) Link the system to a computerized chemical property data base so that certain other inputs may be automatically retrieved (if available).

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3. Personal Communication, a "Publishing Agreement" between Arthur D. Little, Inc. (Cambridge, MA) and McGraw-Hill Book Co. (New York, NY) dated October 10, 1980. Supplementary Provision 14(d) provided in a subsequent personal communication to W. Lyman (A.D. Little, Inc.) dated February 10, 1981.

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8. LIST OF PUBLICATIONS

The following publication was supported by the contract covering Phase III of this program:

Lyman, W.J., Reehl, W.F. and Rosenblatt, D.H. (eds.), Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Co., New York, 1982.

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